Analytical and Simulation of the phonon spectra inside a sphere

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Abstract: In this work we model the oscillations of an elastic body. Our aim is to achieve the phonon spectra of a sphere. Once we achieved this goal we develop different codes in order to see the behavior of phonons' frequencies with the radius. Later on we study numerically the thermal excitation of this phonons system.

I. INTRODUCTION

The elasticity theory begins in 1679 with Hooke's Law and continues with different contributions such as those of Jacob Bernoulli(1705), Daniel Bernoulli(1742), L. Euler with *elastica*(1744), Navier(1821) and the studies of Cauchy about stress, non-linear and linear elasticity(1822). Later on more advances in non-linear elasticity became important. Refs. [1/4].

In the last decades the oscilations of the phonons became a key in the fields of quantum information and optomechanics as we can see in Ref. [5], or in levitated systems as can be seen in Ref. [6]. They also became crucial in complicated systems such as studying the evolution of temperature of a levitated system as seen in Ref. [7].

To achieve our goal we will fight the problem analytically and then simulate our results with matlab in order to have better conclusions.

II. ELASTICITY THEORY

Linear elasticity theory describes the dynamics of small deformations of a continuous solid body from its equilibrium state. We will detail now the main concepts of elasticity theory briefly, addressing the reader to Refs, [1/4] for further information.

Let our body be a simply connected set $B \subseteq \mathbb{R}^3$ with surface ∂B. We now define the *displacement field* $\mathbf{u}(\mathbf{r}, t)$ as the amplitude and direction of the displacement of each point $\mathbf{r} \in B$ at a given time t. We need the displacement field to be at least twice continuously differentiable and both $\mathbf{u}$ and $\dot{\mathbf{u}}$ need to be square integrable to ensure finite energy of the system, $\mathbf{u}, \dot{\mathbf{u}} \in L^2(B)$.

In order to develop the theory we will need the mass density field $\rho(\mathbf{r})$ and the elasticity tensor field $C(\mathbf{r})$. We will work under the assumptions of: homogeneous elastic body (which implies ρ and C to be constant) and isotropic body, that means our elasticity tensor simplifies to

$$C_{ijkl} = \mu[\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}] + \lambda\delta_{ij}\delta_{kl}. \tag{1}$$

The two coefficients λ, μ are known as *Lamé parameters* or *elasticity coefficients.*

It is useful to define the *strain tensor*

$$\mathbf{E} = \frac{1}{2}[\nabla\mathbf{u} + (\nabla\mathbf{u})^t], \tag{2}$$

in order to characterize the variations in the displacement field, and the *stress tensor field* $\mathbf{S}(\mathbf{r})$ to characterize how much energy is needed to effect this strain. We have the following relation between them

$$\mathbf{S} = \mathbf{C} \cdot \mathbf{E}. \tag{3}$$

We will commonly use the stress tensor field in the direction $\mathbf{j}$ that is written as $\mathbf{s}_j = \mathbf{S} \cdot \mathbf{j}$.

We are interested in the dynamics of the displacement field which is governed by the equation

$$\rho\ddot{\mathbf{u}} = \nabla \cdot [\mathbf{C} \cdot \nabla\mathbf{u}], \tag{4}$$

or using the Euler convention

$$\rho\ddot{u}_i = \partial^j C_{ijkl}\partial^k u^l. \tag{5}$$

We can define the differential operator D as

$$D\mathbf{u} = \nabla \cdot [\mathbf{C} \cdot \nabla\mathbf{u}],$$

so we get the equation of motion in a more compact form

$$\rho\ddot{\mathbf{u}} = D\mathbf{u}.$$

As we will work under the assumption of a *free body* it will satisfy the pure Neumann boundary condition

$$\mathbf{s}_j(\mathbf{r}, t) = 0 \quad \forall\mathbf{r} \in \partial B. \tag{6}$$

With the initial values and this boundary condition it can be proven that the problem has at most one solution [3].

Taking into account that in our problem we have an homogeneous elastic body with constant density and elasticity tensor with the boundary conditions (6) we simplify our equation of motion to

$$\begin{aligned} D\mathbf{u} &= \mathbf{C} \cdot \nabla\nabla\mathbf{u} \\ [D\mathbf{u}]_i &= C_{ijkl}\partial^j\partial^k u^l. \end{aligned} \tag{7}$$

The main problem reduces now to find eigenfunctions $\mathbf{w}(\mathbf{r})$ of the differential operator D with eigenvalue d

$$D\mathbf{w}_n(\mathbf{p}; \mathbf{r}) = d_n(\mathbf{p})\mathbf{w}_n(\mathbf{p}; \mathbf{r}). \tag{8}$$

Where n is a discrete multi-index and $\mathbf{p}$ is a continuous multi-index that we will use to label the different eigenfunctions, in $\mathbf{p}$ is represented the effect of how the energy change continuously with the radius R, and on n we will label the different eigenfunctions for the same $\mathbf{p}$. From now on we will call these eigenfunctions the eigenmodes of our system.

Once we obtain the eigenmodes if we make the canonical quantization we obtain the Hamilton operator

$$\hat{H} = \sum_n \int d\mathbf{p} \hbar \omega_n \hat{a}_n^\dagger(\mathbf{p}) \hat{a}_n(\mathbf{p}), \tag{9}$$

where $\hat{a}_n$ and $\hat{a}_n^\dagger$ are the *ladder operators* who satisfies the canonical commutations relations

$$\left[\hat{a}_n(\mathbf{p}), \hat{a}_m^\dagger(\mathbf{p}')\right] = \delta_{nm}\delta(\mathbf{p}-\mathbf{p}'). \tag{10}$$

III. ANALYTICAL SOLUTION

We now consider a free linear elastic, homogeneous, isotropic sphere of radius R

$$B = \{(r,\theta,\varphi) \,| 0 \le r \le R, 0 \le \varphi < 2\pi, 0 \le \theta \le \pi\}, \tag{11}$$
$$\partial B = \{(R,\theta,\varphi) \,| 0 \le \varphi < 2\pi, 0 \le \theta \le \pi\}. \tag{12}$$

Like we have seen before to obtain its quantized phonon field, we have to determine the classical eigenmodes by solving the eigenvalue equation with its boundary conditions(equations (6) and (8)). We will obtain the general form of the eigenmodes in spherical coordinates, and then enforce the boundary conditions in a second step.

A. Solution of eigenvalue equation

We start by expressing the displacement field as

$$\mathbf{u}(\mathbf{r},t) = \vec{\nabla} f(\mathbf{r},t) + \vec{\nabla} \times \Psi(\mathbf{r},t), \tag{13}$$

where $f(\mathbf{r},t)$ is the *scalar potential* and $\Psi(\mathbf{r},t)$ is the *vector potential.* Note that we can always decompose a vector field as in Eq. (13) as proven in Ref. [1]. We now express the eigenmodes $\mathbf{w}$ through potentials

$$\mathbf{w}(\mathbf{r}) = \vec{\nabla} f(\mathbf{r}) + \vec{\nabla} \times \Psi(\mathbf{r}), \tag{14}$$

and insert it into Eq. (8) to obtain

$$\Delta f(\mathbf{r}) = -\frac{\omega^2}{c_L^2} f(\mathbf{r}), \tag{15}$$

$$\Delta \Psi(\mathbf{r}) = -\frac{\omega^2}{c_T^2} \Psi(\mathbf{r}), \tag{16}$$

where we have defined the *longutidunal and transverse speed of sound*

$$c_L = \sqrt{\frac{2\mu+\lambda}{\rho}}; \qquad c_T = \sqrt{\frac{\mu}{\rho}}. \tag{17}$$

These velocities are only a function of density ρ and the two elasticity coefficients μ and λ.

From now on we will work with spherical coordinates and we will express $\Psi = \left(\Psi^r, \Psi^\theta, \Psi^\varphi\right)$. In this coordinate system, Eq. (16) can be expanded into a set of three coupled equations using the common Gauge condition $\Delta\Psi = 0$, these set of equations is problematic to solve since uncoupling it is very difficult. In order to solve this problem we make use of Ref. [4] where we find a new expression for $\mathbf{\Psi}$ and a new Gauge condition that appear naturally to simplify your equations once you start solving them. In spherical coordinates, let $\mathbf{\Psi}$ be

$$\mathbf{\Psi} = r\Psi\mathbf{e_r} + \nabla \times (r\zeta\mathbf{e_r}). \tag{18}$$

Now we will impose and solve the Gauge condition

$$\nabla \times \left[\nabla^2 (r\Psi\mathbf{e_r}) - \frac{r}{c_T^2}\ddot{\Psi}\mathbf{e_r}\right] = 0. \tag{19}$$

Using properties of spherical Bessel functions we obtain

$$f(r,\theta,\varphi) = Aj_l(Mr)\,Y_l^m(\theta,\varphi), \tag{20}$$
$$\Psi(r,\theta,\varphi) = Bj_l(Qr)\,Y_l^m(\theta,\varphi), \tag{21}$$
$$\zeta(r,\theta,\varphi) = Cj_l(Qr)Y_l^m(\theta,\varphi), \tag{22}$$

where $M = \frac{\omega}{c_L}$, $Q = \frac{\omega}{c_T}$, $j_l(z)$ is the spherical Bessel function, $Y_l^m(\theta,\varphi)$ is the spherical harmonic function and A, B and C are the free amplitudes.

Once we arrive to this point expressing $\mathbf{w}$ in spherical coordinates, $\mathbf{w} = (W^r, W^\theta, W^\varphi)$ we obtain the solutions (using equation (14))

$$\begin{aligned} W^r = AMj_l'(Mr)Y_l^m + \frac{Cj_l(Qr)}{r}\Bigg[&-\frac{cos\theta}{sin\theta}\frac{\partial}{\partial\theta}Y_l^m \\ &-\frac{\partial^2}{\partial\theta^2}Y_l^m + \frac{m^2}{sin^2\theta}Y_l^m\Bigg], \end{aligned} \tag{23}$$

$$\begin{aligned} W^\theta = {}& \frac{A}{r}j_l(Mr)\frac{\partial}{\partial\theta}Y_l^m + \frac{Bim}{sin\theta}j_l(Qr)Y_l^m \\ &+ \frac{Cj_l(Qr)}{r}\frac{\partial}{\partial\theta}Y_l^m + QCj_l'(Qr)\frac{\partial}{\partial\theta}Y_l^m, \end{aligned} \tag{24}$$

$$\begin{aligned} W^\varphi = {}& \frac{Aim}{rsin\theta}j_l(Mr)Y_l^m - Bj_l(Qr)\frac{\partial}{\partial\theta}Y_l^m \\ &+ \frac{Cim}{rsin\theta}j_l(Qr)Y_l^m + \frac{CQim}{sin\theta}j_l'(Qr)Y_l^m, \end{aligned} \tag{25}$$

where we used the notation $j_l'(z) = \frac{\partial}{\partial z}j_l(z)$.

B. Stress-free boundary condition

The second step is to calculate the stress matrix terms in spherical coordinates, from the relation in cartesian coordinates

$$S_{ij} = \mu(\partial_i u_j + \partial_j u_i) + \lambda\delta_{ij}\partial_k u^k. \tag{26}$$

In order to implement the boundary conditions we need to calculate the stress vector field of the eigendomdes on the sphere surface, i.e. $\mathbf{s_j}$ with $\mathbf{j} = \mathbf{e_r}$

$$\mathbf{S e_r} = \mathbf{S_r} = (s^r, s^\theta, s^\varphi), \tag{27}$$

we need to express the spherical stress matrix in terms of the cartesian ones. After using the displacement field in spherical coordinates $\mathbf{u}=(u^r, u^\theta, u^\varphi)$ we obtain

$$s^r = 2\mu\partial_r u^r + \lambda\vec{\nabla}\vec{u} = 2\mu\left(\partial_r u^r + \frac{f\omega^2}{2}\left(\frac{2}{c_L^2} - \frac{1}{c_T^2}\right)\right), \tag{28}$$

$$s^\theta = \mu\left[\frac{\partial u^\theta}{\partial r} + \frac{1}{r}\left(\frac{\partial u^r}{\partial\theta} - u^\theta\right)\right], \tag{29}$$

$$s^\varphi = \mu\left[\frac{\partial u^\varphi}{\partial r} + \frac{1}{r}\left(\frac{\partial u^r}{\partial\varphi} - u^\varphi\right)\right]. \tag{30}$$

We can write these equations at the surface of the sphere.

$$s^r(R,\theta,\varphi) = 2\mu\left(D_{11}A + D_{12}B + D_{13}C\right), \tag{31}$$

$$s^\theta(R,\theta,\varphi) = \mu\left(D_{21}A + D_{22}B + D_{23}C\right), \tag{32}$$

$$s^\varphi(R,\theta,\varphi) = \mu\left(D_{31}A + D_{32}B + D_{33}C\right). \tag{33}$$

Where the corresponding matrix elements are

$$D_{11} = \frac{\partial^2}{\partial r^2}f + \frac{fw^2}{2}\left(\frac{2}{c_L^2} - \frac{1}{c_T^2}\right), \tag{34}$$

$$D_{12} = 0, \tag{35}$$

$$D_{13} = \frac{\partial}{\partial r}\left[-\frac{1}{rsin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\zeta\right) - \frac{1}{rsin^2\theta}\frac{\partial^2}{\partial\varphi^2}\zeta\right], \tag{36}$$

$$D_{21} = \frac{2}{r}\frac{\partial^2}{\partial\theta\partial r}f - \frac{2}{r^2}\frac{\partial}{\partial\theta}f, \tag{37}$$

$$D_{22} = \frac{1}{sin\theta}\frac{\partial^2}{\partial r\partial\varphi}\Psi - \frac{1}{rsin\theta}\frac{\partial}{\partial\varphi}\Psi, \tag{38}$$

$$D_{23} = \frac{\partial^3}{\partial r^2\partial\theta}\zeta - \frac{2}{r^2}\frac{\partial}{\partial\theta}\zeta + \frac{1}{r}\frac{\partial}{\partial\theta}\left[-\frac{1}{rsin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\zeta\right) - \frac{1}{rsin^2\theta}\frac{\partial^2}{\partial\varphi^2}\zeta\right], \tag{39}$$

$$D_{31} = \frac{\partial}{\partial r}\left[\frac{1}{rsin\theta}\frac{\partial}{\partial\varphi}f\right] + \frac{1}{r}\frac{\partial^2}{\partial r\partial\varphi}f - \frac{1}{r^2 sin\theta}\frac{\partial}{\partial\varphi}f, \tag{40}$$

$$D_{32} = -\frac{\partial^2}{\partial\theta\partial r}\Psi + \frac{1}{r}\frac{\partial}{\partial\theta}\Psi, \tag{41}$$

$$D_{33} = \frac{1}{sin\theta}\left[\frac{\partial^3}{\partial\varphi\partial r^2}\zeta - \frac{2}{r^2}\frac{\partial}{\partial\varphi}\zeta\right] + \frac{1}{r}\frac{\partial}{\partial\varphi}\left[-\frac{1}{rsin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\zeta\right) - \frac{1}{rsin^2\theta}\frac{\partial^2}{\partial\varphi^2}\zeta\right]. \tag{42}$$

In order to get a nontrivial solution we need the $detD = 0$. This will be the eigenfrequency equation, which is transcendental and cannot be solved analytically.

IV. NUMERICAL CALCULATION

We will now develop a code in matlab in order to calculate the first N frequencies for given values of l,m and R. For that goal we will remove from the D_{ij} the $e^{im\varphi}$ who plays no role in the frequency equation. With levitated nanospheres in mind, we will do the calculations for $10\mu m \leq R \leq 100\mu m$. We will work with our units $L_0 = 10\mu m$ and $T_0 = c_L/L_0$. For our simulation we will use Silica because it is a material used nowadays for this type of experiments as we can see in Ref. [7].

First of all we substitute the values of f, ζ and Ψ in the matrix coefficients and express all the Legendre polynomials and spherical Bessel functions in terms of degrees l and l+1. Doing this we are able to take out common terms of some rows or columns in order to simplify the determinant. At this point we realize that it is useful (mostly for the code part) to study three different cases.

A. Case 1:l=0 and m=0

In this case we only have one matrix element different from 0:

$$D_{11} = M^2\left[\left[-1 + \frac{(c_L)^2}{2}\left(\frac{2}{c_L^2} - \frac{1}{c_T^2}\right)\right]j_0(MR) + \frac{2}{MR}j_1(MR)\right]. \tag{43}$$

The boundary condition requires $B = C = 0$ and $D_{11} = 0$ leaving A as the free amplitude we obtain

$$W^r = -Aj_1(\omega R/c), \tag{44}$$

$$W^\theta = 0, \tag{45}$$

$$W^\varphi = 0. \tag{46}$$

This solution is known as the breathing mode, as we only have displacement field in r direction. We can see in figure (1) the values of the frequency that erased the determinant in function of R.

B. Case 2:$l \neq 0$ and m=0

In this case we have $D_{31} = D_{33} = 0$ so the determinant becomes

$$-D_{32} \cdot detM', \tag{47}$$

where $D' = \begin{bmatrix} D_{11} & D_{13} \\ D_{21} & D_{23} \end{bmatrix}$. The determinant can therefore be canceled out in two independent ways, $D_{32} = 0$ or $detD' = 0$. In the first one the boundary condition requires $A = C = 0$ and leaving B as the free amplitude

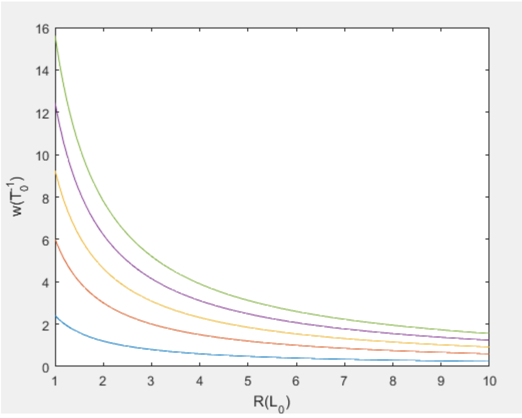

FIG. 1: Eigenvalues of the frequency ω in function of R for l=m=0

we obtain

$$W^r = 0, \tag{48}$$

$$W^\theta = 0, \tag{49}$$

$$W^\varphi = B\frac{j_l(Qr)}{sin\theta}(l+1)\left[cos\theta P_l^0 - P_{l+1}^0\right]. \tag{50}$$

We will call that family the $\varphi_{paralel}$ family. In the second one the boundary conditions require $B = 0$, and we have a free amplitude A and a relation of $C = A(\omega)$.

$$\begin{aligned} W^r = {} & AM\left[\frac{l}{Mr}j_l(Mr) - j_{l+1}(Mr)\right]Y_l^0 \\ & + \frac{Cj_l(Qr)}{r}l(l+1)Y_l^0, \end{aligned} \tag{51}$$

$$\begin{aligned} W^\theta = {} & \frac{l+1}{r}\left[Aj_l(Mr) + QC\left[\frac{l+1}{Qr}j_l(Qr) - j_{l+1}(Qr)\right]\right] \\ & \left[-cos\theta P_l^0 + P_{l+1}^0\right], \end{aligned} \tag{52}$$

$$W^\varphi = 0. \tag{53}$$

That we named $\varphi_{perpendicular}$ family. If we plot for l=1 this two cases we obtain figures (2) and (3).

C. Case 3: $m \neq 0$

In this case we have the whole determinant and the solution we discussed before (equations (23-25)). We will show the graphic for one example in order to see its behavior in fig (4).

V. DEPENDENCE WITH THE SPHERE RADIUS

Studying the different plots(the ones that we showed here and so many others) we realized that the frequency has a behavior of

$$\omega(R) \quad \propto \quad \frac{1}{R}. \tag{54}$$

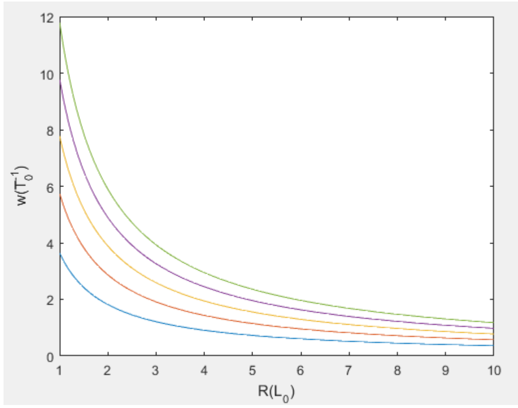

FIG. 2: Eigenvalues of the frequency ω as a function of R for m=0 and l=1 φcomponent family

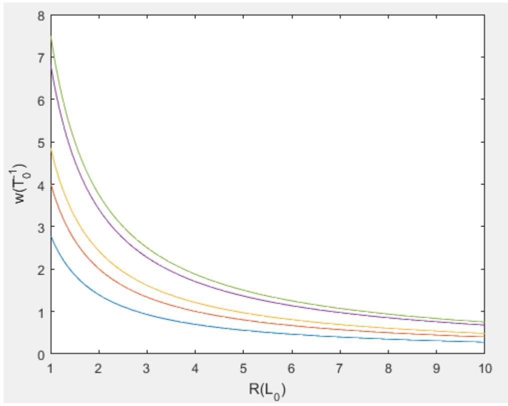

FIG. 3: Eigenvalues of the frequency ω as a function of R for m=0 and l=1 φcomponent= 0 family

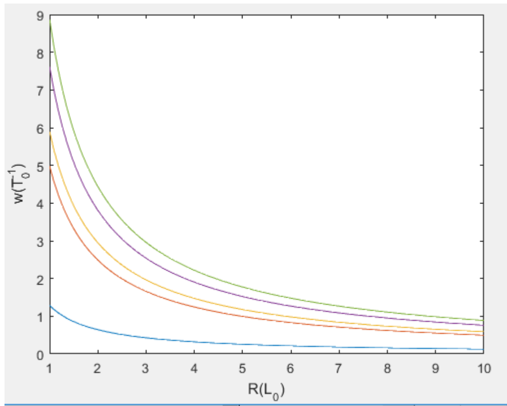

FIG. 4: Eigenvalues of the frequency ω as a function of R for m=-1 l=2 $\theta = \pi/8$

We can demonstrate this by doing this change of variables $x = \omega R$. Then for a given material we have c_L and c_T constants. After that for a given value of l, m and θ we obtain that all the matrix coefficients are a function of x. Therefore, we conclude that as the coefficients are composed by oscillating functions they will have different values of x that erased the determinant. We can label those zeros as x_n and as $x_n = wR$ the w solutions for a given family n is:

$$\omega_n(R) = \frac{x_n}{R}. \tag{55}$$

We observed too that the x_n values are not θ dependent, although it could be not easy to show analytically.

VI. THERMAL ANALYSIS

Due to the scaling with radius uncovered above, for a nanometric sphere, not many phonon modes will be occupied at low temperatures. Since this is a potential advantage for quantum applications, we devote this section to calculate the number of states that are below the thermal frequency and have less l than a given one. The definition of the thermal frequency is

$$\omega_{th} = \frac{k_B T}{\hbar}.$$

Studying numerically these cases we realize that for a given l the state of less frequency is m=-l. In figure 5, we see the modes excited with l less or equal to 35 and $R = 10^{-6}m$. We notice that for T lower than a certain value the occupation is in average less than 1 phonon. This is useful for quantum applications where, in analogy with quantum optics, the generation of a single excitation state is key. This temperature is remarkably reachable for most cryogenic setups.

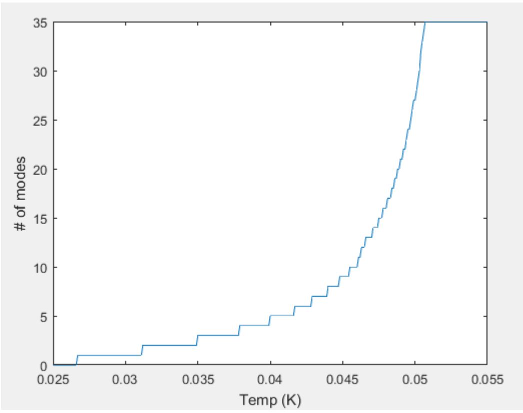

FIG. 5: Modes excited with $l \leq 35$ with $R = 10^{-6}m$ as a function of T

VII. CONCLUSIONS

We have developed a model for the phonons in a given body. With this model we have achieved the expression of the eigenmodes in spherical coordinates. Later on we applied it to the case of a sphere with a given radius and material being able to find the quantum acoustic modes. We have proved that the radius and frequency are inversely proportional and we have been able to label the frequency spectra.

Numerically we have achieved multiples codes in order to calculate the different eigenvalues of our frequency and to study the excitation of these modes with temperature.

An important point is that we have temperatures lower than a certain value in which the average of phonons is less than one. This point is key in order to generate a single excitation state. Therefore this temperature is remarkably reachable for most cryogenic setups so it would be an interesting field of study.

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